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Evolution of Magnetic Moments in Cobalt and Nickel Clusters[1]
MASAHIRO SAKURAI, JAIME SOUTO-CASARES, JAMES CHELIKOWSKY, University of Texas at Austin — Ferromagnetism in transition-metal clusters has attracted much interest owing to their enhanced magnetic moments as compared to those of bulk phases. Here, we investigate the stability and the magnetism of Co and Ni clusters with various structures using a real-space formalism of pseudopotentials within the spin-polarized density-functional theory, i.e., the PARSEC code. We will discuss how the calculated magnetic moments evolve as a function of cluster size and compare them to experiment.

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